Connecting via Winsock to STN STN SEARCH

10/560,577

Welcome to STN International! Enter x:x

[illegible]

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page for STN Seminar Schedule - N. America
NEWS 2	MAY 01	New CAS web site launched
NEWS 3	MAY 08	CA/CAplus Indian patent publication number format defined
NEWS 4	MAY 14	RDISCLOSURE on STN Easy enhanced with new search and display fields
NEWS 5	MAY 21	BIOSIS reloaded and enhanced with archival data
NEWS 6	MAY 21	TOXCENTER enhanced with BIOSIS reload
NEWS 7	MAY 21	CA/CAplus enhanced with additional kind codes for German patents
NEWS 8	MAY 22	CA/CAplus enhanced with IPC reclassification in Japanese patents
NEWS 9	JUN 27	CA/CAplus enhanced with pre-1967 CAS Registry Numbers
NEWS 10	JUN 29	STN Viewer now available
NEWS 11	JUN 29	STN Express, Version 8.2, now available
NEWS 12	JUL 02	LEMBASE coverage updated
NEWS 13	JUL 02	LMEDLINE coverage updated
NEWS 14	JUL 02	SCISEARCH enhanced with complete author names
NEWS 15	JUL 02	CHEMCATS accession numbers revised
NEWS 16	JUL 02	CA/CAplus enhanced with utility model patents from China
NEWS 17	JUL 16	CAplus enhanced with French and German abstracts
NEWS 18	JUL 18	CA/CAplus patent coverage enhanced
NEWS 19	JUL 26	USPATFULL/USPAT2 enhanced with IPC reclassification
NEWS 20	JUL 30	USGENE now available on STN
NEWS 21	AUG 06	CAS REGISTRY enhanced with new experimental property tags
NEWS 22	AUG 06	BEILSTEIN updated with new compounds
NEWS 23	AUG 06	FSTA enhanced with new thesaurus edition
NEWS 24	AUG 13	CA/CAplus enhanced with additional kind codes for granted patents
NEWS 25	AUG 20	CA/CAplus enhanced with CAS indexing in pre-1907 records
NEWS 26	AUG 27	Full-text patent databases enhanced with predefined patent family display formats from INPADOCDB
NEWS 27	AUG 27	USPATOLD now available on STN
NEWS 28	AUG 28	CAS REGISTRY enhanced with additional experimental spectral property data

NEWS EXPRESS 29 JUNE 2007: CURRENT WINDOWS VERSION IS V8.2, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 05 JULY 2007.

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 13:56:07 ON 29 AUG 2007

=>
Uploading
THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE
Do you want to switch to the Registry File?
Choice (Y/n):
Switching to the Registry File...
Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> FILE REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 13:56:30 ON 29 AUG 2007
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 28 AUG 2007 HIGHEST RN 945714-55-6
DICTIONARY FILE UPDATES: 28 AUG 2007 HIGHEST RN 945714-55-6

New CAS Information Use Policies, enter HELP USAGETERMS for details.

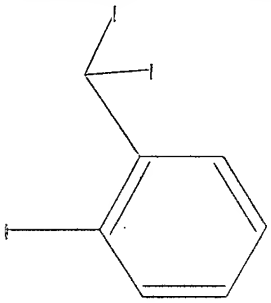
TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

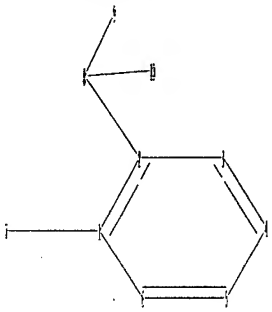
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10560577.str





chain nodes :

```
7  8  9  10
ring nodes :
1  2  3  4  5  6
chain bonds :
1-7  2-8  8-9  8-10
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6
exact/norm bonds :
1-7
exact bonds :
2-8  8-9  8-10
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6
isolated ring systems :
containing 1 :

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:CLASS  8:CLASS  9:CLASS  10:CLASS



L1      STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1                STR
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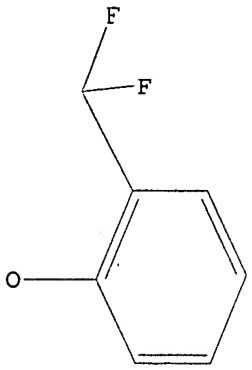


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Structure attributes must be viewed using STN Express query preparation.


=> s l1
SAMPLE SEARCH INITIATED 13:56:44 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     2220 TO ITERATE

 90.1% PROCESSED     2000 ITERATIONS                                 50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        41574 TO    47226
PROJECTED ANSWERS:            9624 TO    12442

L2            50 SEA SSS SAM L1

=> s l1 sss full
FULL SEARCH INITIATED 13:57:08 FILE 'REGISTRY'
```

FULL SCREEN SEARCH COMPLETED - 45450 TO ITERATE

100.0% PROCESSED 45450 ITERATIONS 10842 ANSWERS
SEARCH TIME: 00.00.01

L3 10842 SEA SSS FUL L1

=> FIL CAPLUS
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 172.10 172.31

FILE 'CAPLUS' ENTERED AT 13:57:15 ON 29 AUG 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 29 Aug 2007 VOL 147 ISS 10
FILE LAST UPDATED: 28 Aug 2007 (20070828/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

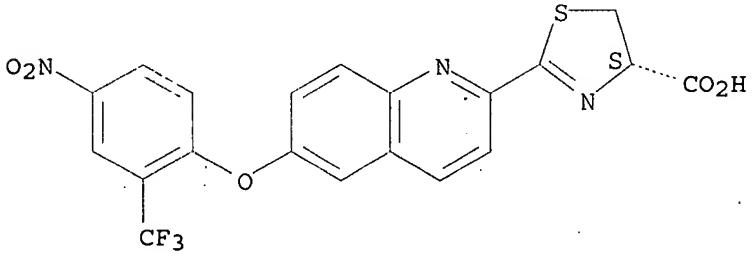
=> s l3
L4 2663 L3

=> s l4 and (reporter or label or dye? or chromophore or fluorophore or cyanine or rhodamine or fluoresceine)
51449 REPORTER
2062 REPORTERS
52598 REPORTER
(REPORTER OR REPORTERS)
65886 LABEL
23008 LABELS
79274 LABEL
(LABEL OR LABELS)
392055 DYE?
26449 CHROMOPHORE
19197 CHROMOPHORES
37209 CHROMOPHORE
(CHROMOPHORE OR CHROMOPHORES)
8243 FLUOROPHORE
4980 FLUOROPHORES
11449 FLUOROPHORE
(FLUOROPHORE OR FLUOROPHORES)
15873 CYANINE
1412 CYANINES
16298 CYANINE
(CYANINE OR CYANINES)
22074 RHODAMINE
587 RHODAMINES
22230 RHODAMINE

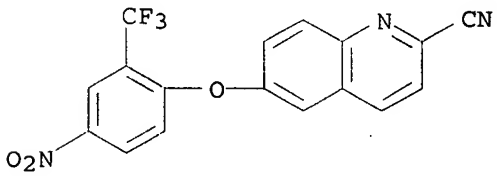
```
                (RHODAMINE OR RHODAMINES)
            161 FLUORESCEINE
              1 FLUORESCEINES
            161 FLUORESCEINE
                (FLUORESCEINE OR FLUORESCEINES)
L5           78 L4 AND (REPORTER OR LABEL OR DYE? OR CHROMOPHORE OR FLUOROPHORE
                OR CYANINE OR RHODAMINE OR FLUORESCEINE)

=> s l5 and enzyme
         825251 ENZYME
         469820 ENZYMES
        1039299 ENZYME
                (ENZYME OR ENZYMES)
L6            6 L5 AND ENZYME

=> d l6 ibib abs hitstr tot

L6   ANSWER 1 OF 6  CAPLUS  COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:         2006:1279865  CAPLUS
DOCUMENT NUMBER:          146:57589
TITLE:                    Luminogenic and fluorogenic compounds and methods to
                          detect molecules or conditions
INVENTOR(S):              Daily, William; Hawkins, Erika; Klaubert, Dieter; Liu,
                          Jianquan; Meisenheimer, Poncho; Scurria, Michael;
                          Shultz, John W.; Unch, James; Wood, Keith V.; Zhou,
                          Wenhui; Valley, Michael P.; Cali, James J.
PATENT ASSIGNEE(S):       Promega Corporation, USA
SOURCE:                   PCT Int. Appl., 328pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.           KIND   DATE       APPLICATION NO.          DATE
     ---------------      ----   --------   ---------------------    --------
     WO 2006130551         A2    20061207   WO 2006-US20731          20060530
     WO 2006130551         A8    20070201
     WO 2006130551         A3    20070503
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR,
             KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX,
             MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE,
             SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC,
             VN, YU, ZA, ZM, ZW
         RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
             IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
             CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
             GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA
     US 2007015790         A1    20070118   US 2006-444145           20060531
PRIORITY APPLN. INFO.:                      US 2005-685957P      P   20050531
                                            US 2005-693034P      P   20050621
                                            US 2005-692925P      P   20050622
                                            US 2006-790455P      P   20060407
OTHER SOURCE(S):          MARPAT 146:57589
AB   A method to detect the presence or amount of at least one mol. in a sample
     which employs a derivative of luciferin or a derivative of a fluorophore
     is provided.
IT   916661-05-7P
     RL: BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL
     (Biological study); PREP (Preparation); USES (Uses)
        (luminogenic and fluorogenic compds. and methods to detect mols. or
        conditions)
```

RN 916661-05-7 CAPLUS
CN 4-Thiazolecarboxylic acid, 4,5-dihydro-2-[6-[4-nitro-2-(trifluoromethyl)phenoxy]-2-quinolinyl]-, (4S)- (CA INDEX NAME)

Absolute stereochemistry.



IT 916661-06-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(luminogenic and fluorogenic compds. and methods to detect mols. or conditions)
RN 916661-06-8 CAPLUS
CN 2-Quinolinecarbonitrile, 6-[4-nitro-2-(trifluoromethyl)phenoxy]- (CA INDEX NAME)



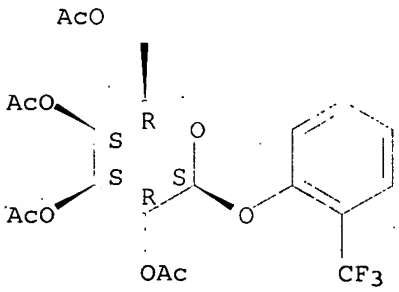
L6 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:1301834 CAPLUS
DOCUMENT NUMBER: 144:102745
TITLE: Synthesis and evaluation of novel enhanced gene reporter molecules: Détection of β-galactosidase activity using 19F NMR of trifluoromethylated aryl β-D-galactopyranosides
AUTHOR(S): Yu, Jianxin; Liu, Li; Kodibagkar, Vikram D.; Cui, Weina; Mason, Ralph P.
CORPORATE SOURCE: Department of Radiology, The University of Texas Southwestern Medical Center at Dallas, Dallas, TX, USA
SOURCE: Bioorganic & Medicinal Chemistry (2006), 14(2), 326-333
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:102745
AB Gene therapy has emerged as a promising strategy for treatment of various diseases, but there is a pressing need for the development of non-invasive reporter techniques based on appropriate mols. and imaging modalities to assay gene expression. The authors now report the design, synthesis, and evaluation of novel enhanced reporter mols., which reveal lacZ gene expression: trifluoromethylated aryl β-D-galactopyranosides. A series of five mol. structures were screened in solution and with stably transfected lacZ expressing human MCF7 breast cancer cells in vitro. P-Trifluoromethyl-o-nitrophenyl β-D-galactopyranoside (PCF3ONPG) was found to exhibit valuable properties including a single 19F NMR signal, stability in aqueous solution and with wild type cells, but a chemical shift response to enzyme

cleavage ($\Delta\delta$ = 1.14 ppm) in breast cancer cells transfected to stably express lacZ.

IT 444-30-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(phase transfer preparation of trifluoromethylated aryl β-D-galactopyranosides and use as 19F NMR reporter mols. for detection of gene lacZ β-galactosidase expression in MCF7 breast cancer cells)
RN 444-30-4 CAPLUS
CN Phenol, 2-(trifluoromethyl)- (CA INDEX NAME)

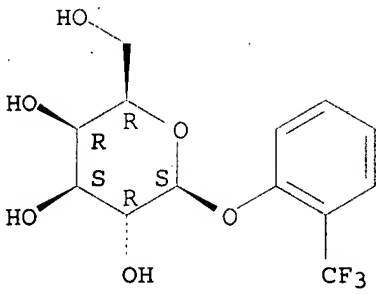
IT 872855-76-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(phase transfer preparation of trifluoromethylated aryl β-D-galactopyranosides and use as 19F NMR reporter mols. for detection of gene lacZ β-galactosidase expression in MCF7 breast cancer cells)
RN 872855-76-0 CAPLUS
CN β-D-Galactopyranoside, 2-(trifluoromethyl)phenyl, tetraacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 872855-81-7P
RL: ARG (Analytical reagent use); BSU (Biological study, unclassified); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); USES (Uses)
(reporter substrate; phase transfer preparation of trifluoromethylated aryl β-D-galactopyranosides and use as 19F NMR reporter mols. for detection of gene lacZ β-galactosidase expression in MCF7 breast cancer cells)
RN 872855-81-7 CAPLUS
CN β-D-Galactopyranoside, 2-(trifluoromethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:858562 CAPLUS
DOCUMENT NUMBER: 142:34367
TITLE: Mechanism-based Fluorescent Labeling of β-Galactosidases: An Efficient Method in Proteomics for Glycoside Hydrolases
AUTHOR(S): Kurogochi, Masaki; Nishimura, Shin-Ichiro; Lee, Yuan Chuan
CORPORATE SOURCE: Division of Biological Sciences, Graduate School of Science, Frontier Research Center for Post-Genomic Science and Technology, Hokkaido University, Sapporo, 001-0021, Japan
SOURCE: Journal of Biological Chemistry (2004), 279(43), 44704-44712
CODEN: JBCHA3; ISSN: 0021-9258
PUBLISHER: American Society for Biochemistry and Molecular Biology
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:34367

AB (4-N-5-Dimethylaminonaphthalene-1-sulfonyl-2-difluoromethylphenyl)-β-D-galactopyranoside was synthesized and successfully tested on β-galactosidases from Xanthomonas manihotis, Escherichia coli, and Bacillus circulans for the rapid identification of the catalytic site. Reaction of the irreversible inhibitor with enzymes proceeded to afford a fluorescence-labeled protein suitable for further high throughput characterization by using antidansyl antibody and matrix-assisted laser desorption ionization time-of-flight/time-of-flight (MALDI-TOF/TOF). Specific probing by a fluorescent aglycon greatly facilitated identification of the labeled peptide fragments from β-galactosidases. It was demonstrated by using X. manihotis β-galactosidase that the Arg-58 residue, which is located within a sequence of 56IPRAYWKD63, was labeled by nucleophilic attack of the guanidinyl group. This sequence including Arg-58 (Leu-46 to Tyr-194) was similar to that (Met-1 to Tyr-151) of Thermus thermophilus A4, which is the first known structure of glycoside hydrolases family 42. A catalytic glutamic acid (Glu-537) of E. coli β-galactosidase was shown to be labeled by the same procedure, suggesting that the modification site with this irreversible substrate might depend both on the nucleophilicity of the amino acids and their spatial arrangement in the individual catalytic cavity. Similarly, a Glu-259 in 257TLEE260 was selectively labeled using B. circulans β-galactosidase, indicating that Glu-259 is one of the nucleophiles in the active site. The present method can be readily extended to other glycosidases and should greatly aid the high throughput proteomics of many glycoside hydrolases showing both retaining- and inverting-type mechanisms.

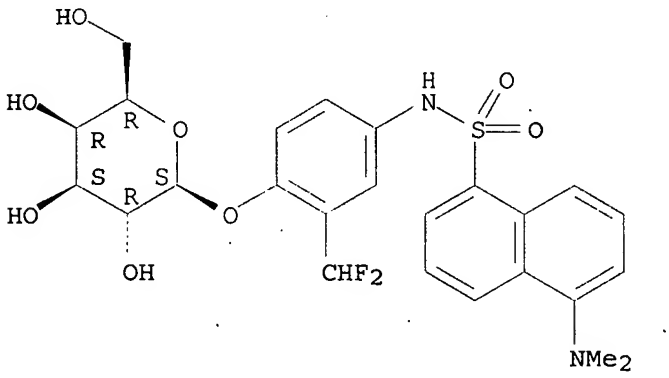
IT 805262-61-7P
RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP

(Preparation); USES (Uses)
(fluorescent label-containing suicide substrate addresses catalytic role of active site Arg and Glu residues in bacterial β-galactosidases)

RN 805262-61-7 CAPLUS

CN 1-Naphthalenesulfonamide, N-[3-(difluoromethyl)-4-(β-D-galactopyranosyloxy)phenyl]-5-(dimethylamino)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



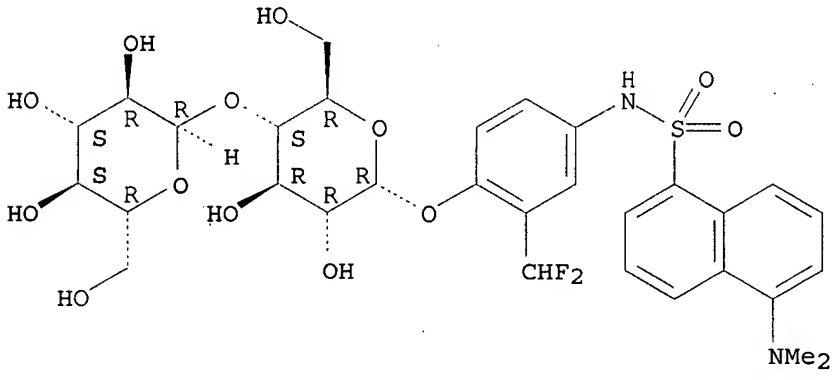
IT 805262-69-5P

RL: PNU (Preparation, unclassified); PREP (Preparation)
(fluorescent label-containing suicide substrate addresses catalytic role of active site Arg and Glu residues in bacterial β-galactosidases)

RN 805262-69-5 CAPLUS

CN 1-Naphthalenesulfonamide, N-[3-(difluoromethyl)-4-[(4-O-α-D-glucopyranosyl-α-D-glucopyranosyl)oxy]phenyl]-5-(dimethylamino)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



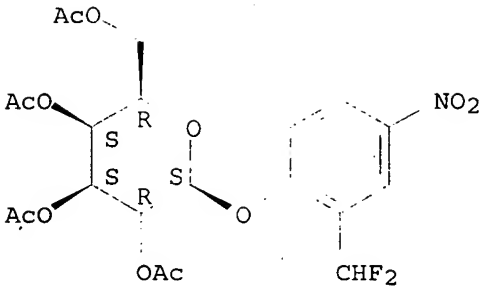
IT 188434-25-5P 328401-17-8P 805262-52-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(fluorescent label-containing suicide substrate addresses catalytic role of active site Arg and Glu residues in bacterial β-galactosidases)

RN 188434-25-5 CAPLUS

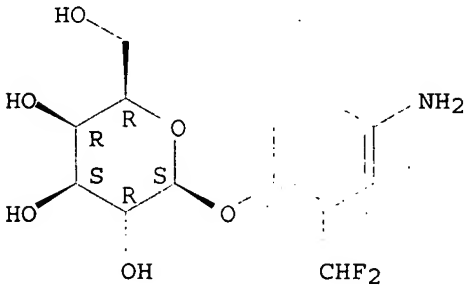
CN β-D-Galactopyranoside, 2-(difluoromethyl)-4-nitrophenyl, 2,3,4,6-tetraacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



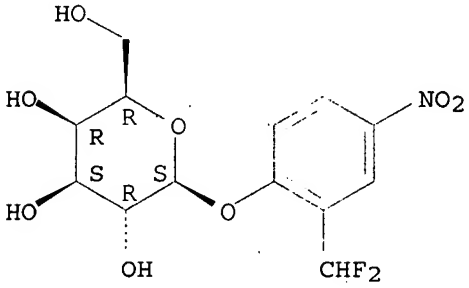
RN 328401-17-8 CAPLUS
CN β-D-Galactopyranoside, 4-amino-2-(difluoromethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 805262-52-6 CAPLUS
CN β-D-Galactopyranoside, 2-(difluoromethyl)-4-nitrophenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

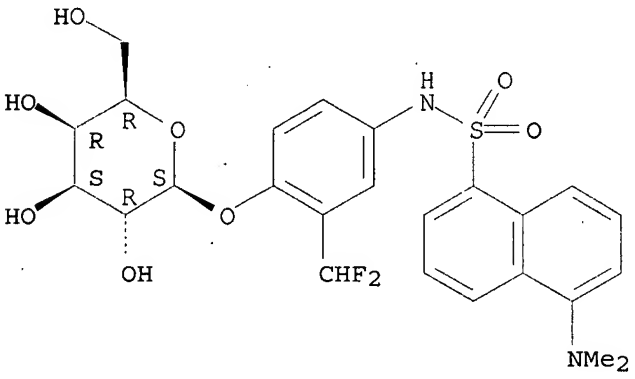
L6 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:314097 CAPLUS
DOCUMENT NUMBER: 142:70626
TITLE: Development of mechanism-based fluorescence affinity labeling reagent for β-galactosidase as proteomics tool: A detailed analysis using MALDI-TOF mass spectrometry
AUTHOR(S): Kurogochi, Masaki; Iwata, Kazumichi; Monde, Kenji; Niikura, Kenichi; Lee, Yuan Chuan; Nishimura, Shin-Ichiro
CORPORATE SOURCE: Division of Biological Sciences, Graduate School of Science, Hokkaido University, Japan
SOURCE: Peptide Science (2003), Volume Date 2004, 40th,

113-114
CODEN: PSCIFQ; ISSN: 1344-7661
PUBLISHER: Japanese Peptide Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB We have prepared mechanism-based fluorescent affinity labeling for useful identification and characterization of β-galactosidase and examined the binding site on β-galactosidase and labeling ability for nucleophile group of enzyme after cleavage of glycoside linkage. We also investigated whether the substance could label various types of β-galactosidase (from Aspergillus oryzae, Escherichia coli., bovine liver, Xanthomonas manihotis, Bacillus circulans) using GPC monitored by fluorescence photometer. All these enzyme could specifically be detected by fluorescence. Then, as for Xanthomonas manihotis, we characterized labeling site of galactosidase via proteomics techniques such as peptide mapping by proteolytic digestion and the followed MS/MS anal. This labeling compound was attached to the side chain of an Arg near the active site.

IT 805262-61-7
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses) (development of mechanism-based fluorescence affinity labeling reagent for β-galactosidase as proteomics tool)
RN 805262-61-7 CAPLUS
CN 1-Naphthalenesulfonamide, N-[3-(difluoromethyl)-4-(β-D-galactopyranosyloxy)phenyl]-5-(dimethylamino)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

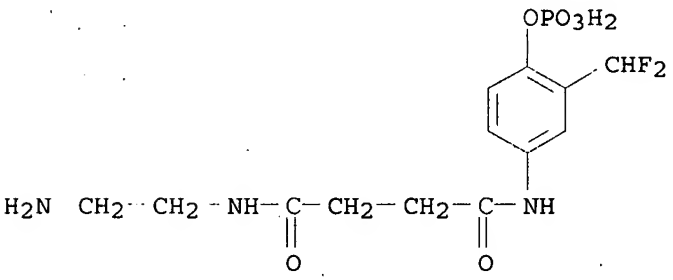
L6 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:190567 CAPLUS
DOCUMENT NUMBER: 139:145678
TITLE: Activity-based fluorescent probes that target phosphatases
AUTHOR(S): Zhu, Qing; Huang, Xuan; Chen, Grace Y. J.; Yao, Shao Q.
CORPORATE SOURCE: Department of Chemistry, National University of Singapore, Singapore, 117543, Singapore
SOURCE: Tetrahedron Letters (2003), 44(13), 2669-2672
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:145678

AB We have successfully designed and synthesized two fluorescently-labeled, activity-based probes, Probe 1 and Probe 2, which were shown to label protein tyrosine phosphatases specifically, as well as other types of phosphatases. The probes were not reactive towards the other

non-phosphatase enzymes tested. These probes may find potential applications in large-scale proteomic expts. whereby subclasses of proteins may be selectively identified.

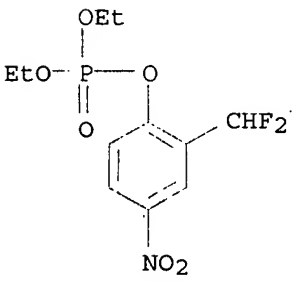
IT 570391-81-0DP, conjugated with Cy3
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(activity-based fluorescent probes that target phosphatases)

RN 570391-81-0 CAPLUS
CN Butanediamide, N-(2-aminoethyl)-N'-[3-(difluoromethyl)-4-(phosphonooxy)phenyl]- (9CI) (CA INDEX NAME)

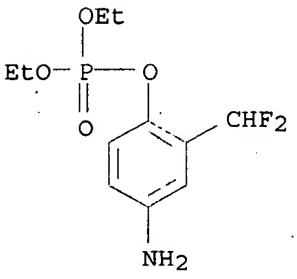


IT 429692-36-4P 429692-37-5P 570391-83-2P
570391-84-3DP, conjugated with Cy3
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(activity-based fluorescent probes that target phosphatases)

RN 429692-36-4 CAPLUS
CN Phosphoric acid, 2-(difluoromethyl)-4-nitrophenyl diethyl ester (9CI) (CA INDEX NAME)

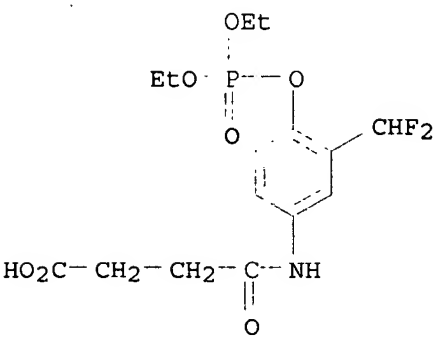


RN 429692-37-5 CAPLUS
CN Phosphoric acid, 4-amino-2-(difluoromethyl)phenyl diethyl ester (9CI) (CA INDEX NAME)

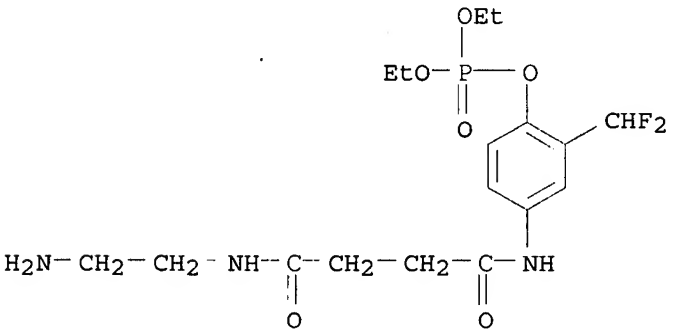


RN 570391-83-2 CAPLUS
CN Butanoic acid, 4-[[4-[(diethoxyphosphinyl)oxy]-3-

(difluoromethyl)phenyl]amino]-4-oxo- (9CI) (CA INDEX NAME)



RN 570391-84-3 CAPLUS
CN Phosphoric acid, 4-[[4-[(2-aminoethyl)amino]-1,4-dioxobutyl]amino]-2-(difluoromethyl)phenyl diethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:790743 CAPLUS
DOCUMENT NUMBER: 130:35356
TITLE: Assays employing electrochemiluminescent labels and electrochemiluminescence quenchers
INVENTOR(S): Richter, Mark M.; Powell, Michael J.; Belisle, Christopher M.
PATENT ASSIGNEE(S): Boehringer Mannheim Corp., USA
SOURCE: PCT Int. Appl., 82 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9853316	A1	19981126	WO 1998-US9552	19980511
W: CA, JP				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
US 2001023063	A1	20010920	US 1998-74472	19980507
CA 2261758	A1	19981126	CA 1998-2261758	19980511
EP 914612	A1	19990512	EP 1998-923375	19980511
EP 914612	B1	20030716		
R: CH, DE, ES, FR, GB, IT, LI				

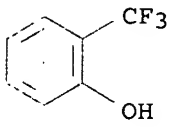
JP 2000517058	T	20001219	JP 1998-550421		19980511
JP 3951031	B2	20070801			
EP 1359416	A2	20031105	EP 2003-15594		19980511
EP 1359416	A3	20040519			
R: CH, DE, ES, FR, GB, IT, LI					
ES 2202860	T3	20040401	ES 1998-923375		19980511
US 2006035248	A1	20060216	US 2005-124407		20050509
PRIORITY APPLN. INFO.:			US 1997-47605P	P	19970523
			US 1998-74472	A3	19980507
			EP 1998-923375	A3	19980511
			WO 1998-US9552	W	19980511

AB This invention pertains to the general field of chemical and biol. assays which employ electrochemiluminescence (ECL), also referred to as electrogenerated chemiluminescence. More particularly, the present invention pertains to certain classes of chemical moieties which strongly quench ECL, and the use of these ECL quenchers in combination with ECL labels, for example, in ECL assay methods which employ an ECL quencher and an ECL label. One class of such quenching moieties are those which comprise at least one benzene moiety. Sub-classes of such quenching moieties are those which comprise at least one phenol moiety, quinone moiety, benzene carboxylic acid, and/or benzene carboxylate moiety.

IT 444-30-4, o-Trifluoromethylphenol
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(assays employing electrochemiluminescent labels and electrochemiluminescence quenchers)

RN 444-30-4 CAPLUS

CN Phenol, 2-(trifluoromethyl)- (CA INDEX NAME)



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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             4 HYDROLYTICS
         44595 HYDROLYTIC
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        825251 ENZYME
        469820 ENZYMES
       1039299 ENZYME
                 (ENZYME OR ENZYMES)
          4392 HYDROLYTIC ENZYME
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L7             0 L4 AND (HYDROLYTIC ENZYME)

=> s l4 and hydrolytic
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         44595 HYDROLYTIC
                 (HYDROLYTIC OR HYDROLYTICS)
L8             4 L4 AND HYDROLYTIC

=> s l8 not l6
L9             4 L8 NOT L6

=> d l9 ibib abs hitstr tot
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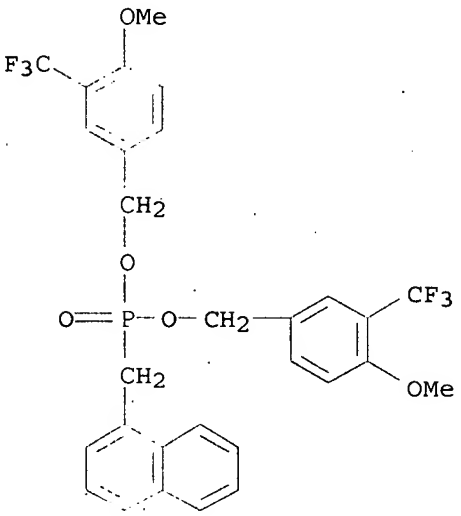
L9 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2007:602620 CAPLUS
DOCUMENT NUMBER: 147:189225
TITLE: Bis[(para-methoxy)benzyl] phosphonate prodrugs with improved stability and enhanced cell penetration
AUTHOR(S): Dang, Qun; Liu, Yan; Rydzewski, Robert M.; Brown, Brian S.; Robinson, Edward; van Poelje, Paul D.; Colby, Timothy J.; Erion, Mark D.
CORPORATE SOURCE: Department of Chemistry, Metabasis Therapeutics, Inc., La Jolla, CA, 92037, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2007), 17(12), 3412-3416
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

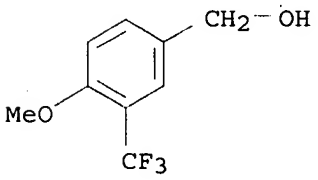
AB A series of substituted bis[(para-methoxy)benzyl] (bisPMB) esters of 1-naphthalenylmethylphosphonic acid (NMPA) were prepared and evaluated as phosphonate prodrugs. Reaction of the 1-naphthylmethylphosphonic dichloridate C10H7CH2POCl2 with benzyl alcs. HOCH2C6H2-3-R1-4-OR2-5-R3 afforded the corresponding diesters, C10H7CH2PO(OCH2C6H2-3-R1-4-OR2-5-R3)2 (4a-m; R2 = Me, Et, Pr; R1 = H, F, Cl, NO2, CN, CF3, Ac, OMe; R3 = H, Cl, Br, OMe), which were tested for their prodrug features by measurement of their half-life times (t1/2) in rat plasma and of intracellular concns. of the free NMPA acid induced by administration of the compds. 4. The prodrug activity is related to facile penetration of the esters through cellular membrane and rapid cytochrome P 450-induced hydrolysis of the phosphonates in the hepatocytes. The esters 4b and 4c with significantly improved aqueous stability were identified that also resulted in increased intracellular levels of NMPA following prodrug incubation with primary rat hepatocytes.

IT 944441-64-9P
RL: BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(preparation of bis-4-methoxybenzyl phosphonates as models for prodrug cell penetration and hydrolytic activation)
RN 944441-64-9 CAPLUS
CN INDEX NAME NOT YET ASSIGNED



IT 261951-88-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of bis-4-methoxybenzyl phosphonates as models for prodrug cell

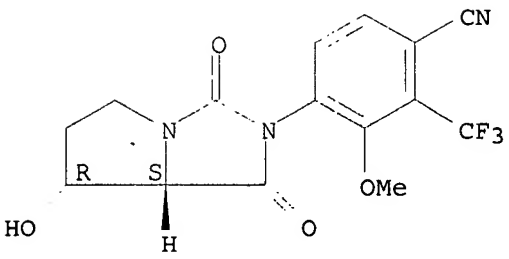
penetration and hydrolytic activation)
RN 261951-88-6 CAPLUS
CN Benzenemethanol, 4-methoxy-3-(trifluoromethyl)- (CA INDEX NAME)



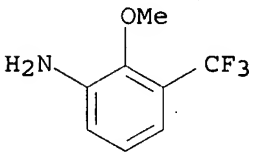
REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2007:267360 CAPLUS
DOCUMENT NUMBER: 146:434187
TITLE: Tandem optimization of target activity and elimination of mutagenic potential in a potent series of N-aryl bicyclic hydantoin-based selective androgen receptor modulators
AUTHOR(S): Hamann, Lawrence G.; Manfredi, Mark C.; Sun, Chongqing; Krystek, Stanley R.; Huang, Yanting; Bi, Yingzhi; Augeri, David J.; Wang, Tammy; Zou, Yan; Betebenner, David A.; Fura, Aberra; Seethala, Ramakrishna; Golla, Rajasree; Kuhns, Joyce E.; Lupisella, John A.; Darienzo, Celia J.; Custer, Laura L.; Price, Jennifer L.; Johnson, James M.; Biller, Scott A.; Zahler, Robert; Ostrowski, Jacek
CORPORATE SOURCE: Pharmaceutical Research Institute, Bristol-Myers Squibb, Princeton, NJ, 08543-5400, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2007), 17(7), 1860-1864
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 146:434187
AB Pharmacokinetic studies in cynomolgus monkeys with a novel prototype selective androgen receptor modulator revealed trace amts. of an aniline fragment released through hydrolytic metabolism This aniline fragment was determined to be mutagenic in an Ames assay. Subsequent concurrent optimization for target activity and avoidance of mutagenicity led to the identification of a pharmacol. superior clin. candidate without mutagenic potential.
IT 627530-78-3P
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(tandem optimization of target activity and elimination of mutagenic potential in series of N-aryl bicyclic hydantoin-based androgen receptor modulators)
RN 627530-78-3 CAPLUS
CN Benzonitrile, 3-methoxy-4-[(7R,7aS)-tetrahydro-7-hydroxy-1,3-dioxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl]-2-(trifluoromethyl)- (CA INDEX NAME)

Absolute stereochemistry.

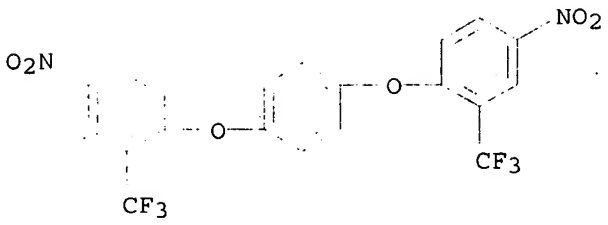


IT 634187-08-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(tandem optimization of target activity and elimination of mutagenic potential in series of N-aryl bicyclic hydantoin-based androgen receptor modulators)
RN 634187-08-9 CAPLUS
CN Benzenamine, 2-methoxy-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

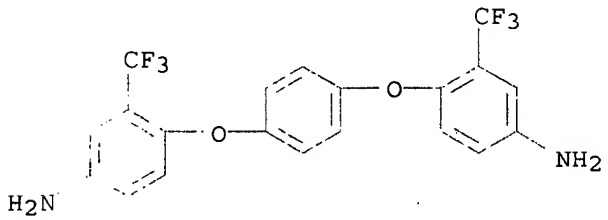


REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

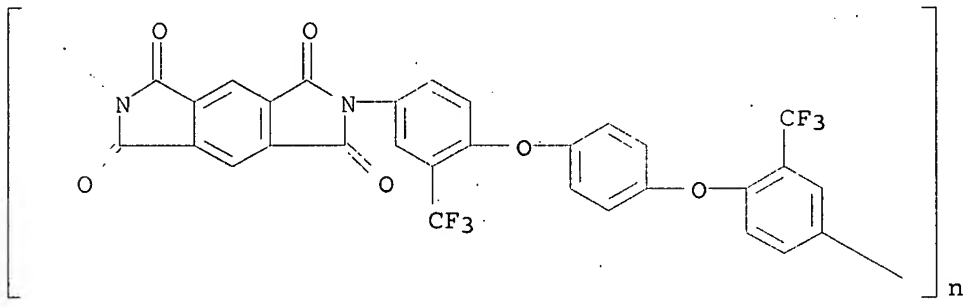
L9 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:32668 CAPLUS
DOCUMENT NUMBER: 134:237921
TITLE: New soluble fluorinated polyimides
AUTHOR(S): Xie, Kun; Zhang, Shu Ying; Liu, Jin Gang; He, Min Hui; Yang, Shi Yong
CORPORATE SOURCE: State Key Laboratory of Engineering Plastics, Center for Molecular Science, Institute of Chemistry, Chinese Academy of Sciences, Beijing, 100080,, Peop. Rep. China
SOURCE: Chinese Chemical Letters (2000), 11(12), 1049-1052
CODEN: CCLEE7; ISSN: 1001-8417
PUBLISHER: Chinese Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The synthesis and properties of a class of soluble fluorine-containing aromatic polyimides are described. The polyimides show desirable features of materials for microelectronics applications.
IT 302781-16-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(monomer synthesis; new soluble fluorinated polyimides)
RN 302781-16-4 CAPLUS
CN Benzene, 1,4-bis[4-nitro-2-(trifluoromethyl)phenoxy]- (CA INDEX NAME)



IT 94525-05-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(monomer; new soluble fluorinated polyimides)
RN 94525-05-0 CAPLUS
CN Benzenamine, 4,4'-[1,4-phenylenebis(oxy)]bis[3-(trifluoromethyl)- (CA INDEX NAME)



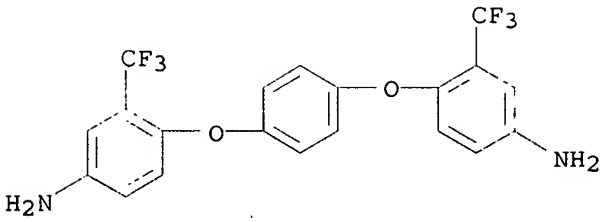
IT 94504-72-0P 94525-06-1P 138283-03-1P
143930-96-5P 302781-17-5P 302781-18-6P
330160-46-8P 330160-47-9P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(new soluble fluorinated polyimides)
RN 94504-72-0 CAPLUS
CN Poly[(5,7-dihydro-1,3,5,7-tetraoxobenzo[1,2-c:4,5-c']dipyrrole-2,6(1H,3H)-diyl)[3-(trifluoromethyl)-1,4-phenylene]oxy-1,4-phenyleneoxy[2-(trifluoromethyl)-1,4-phenylene]] (CA INDEX NAME)



RN 94525-06-1 CAPLUS
CN 1H,3H-Benzo[1,2-c:4,5-c']difuran-1,3,5,7-tetrone, polymer with 4,4'-[1,4-phenylenebis(oxy)]bis[3-(trifluoromethyl)benzenamine] (CA INDEX NAME)

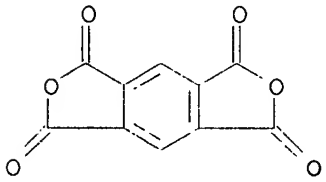
CM 1

CRN 94525-05-0
CMF C20 H14 F6 N2 O2



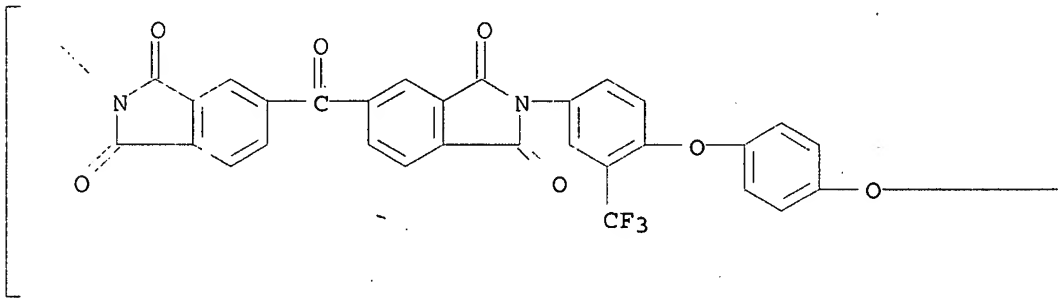
CM 2

CRN 89-32-7
CMF C10 H2 O6

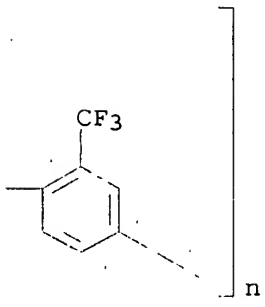


RN 138283-03-1 CAPLUS
CN Poly[(1,3-dihydro-1,3-dioxo-2H-isoindole-2,5-diyl)carbonyl(1,3-dihydro-1,3-dioxo-2H-isoindole-5,2-diyl)[3-(trifluoromethyl)-1,4-phenylene]oxy-1,4-phenyleneoxy[2-(trifluoromethyl)-1,4-phenylene]] (9CI) (CA INDEX NAME)

PAGE 1-A



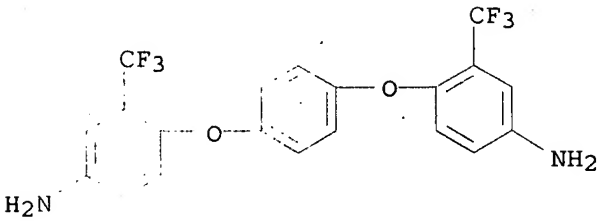
PAGE 1-B



RN 143930-96-5 CAPLUS
CN 1,3-Isobenzofurandione, 5,5'-carbonylbis-, polymer with 4,4'-[1,4-phenylenebis(oxy)]bis[3-(trifluoromethyl)benzenamine] (9CI) (CA INDEX NAME)

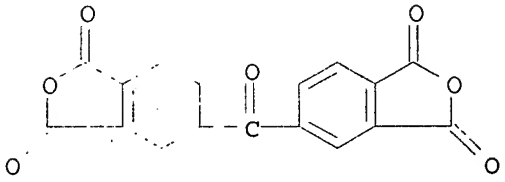
CM 1

CRN 94525-05-0
CMF C20 H14 F6 N2 O2



CM 2

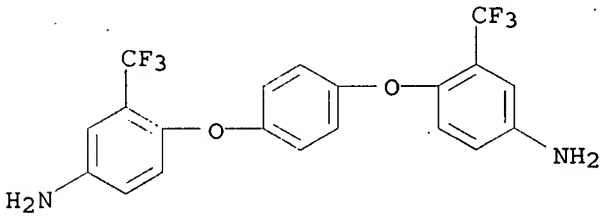
CRN 2421-28-5
CMF C17 H6 O7



RN 302781-17-5 CAPLUS
CN 1,3-Isobenzofurandione, 5,5'-[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]bis-, polymer with 4,4'-[1,4-phenylenebis(oxy)]bis[3-(trifluoromethyl)benzenamine] (CA INDEX NAME)

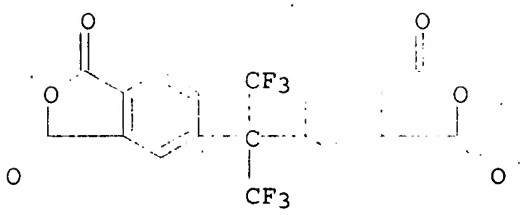
CM 1

CRN 94525-05-0
CMF C20 H14 F6 N2 O2



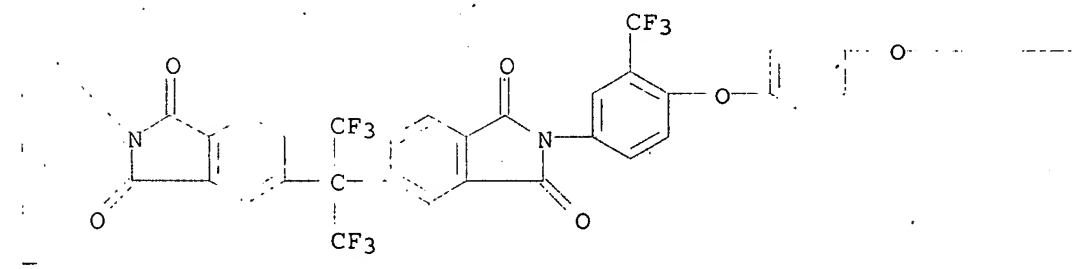
CM 2

CRN 1107-00-2
CMF C19 H6 F6 O6

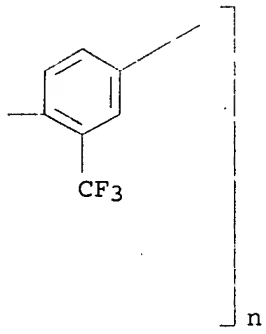


RN 302781-18-6 CAPLUS
CN Poly[(1,3-dihydro-1,3-dioxo-2H-isoindole-2,5-diyl)[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene](1,3-dihydro-1,3-dioxo-2H-isoindole-5,2-diyl)[3-(trifluoromethyl)-1,4-phenylene]oxy-1,4-phenyleneoxy[2-(trifluoromethyl)-1,4-phenylene]] (CA INDEX NAME)

PAGE 1-A



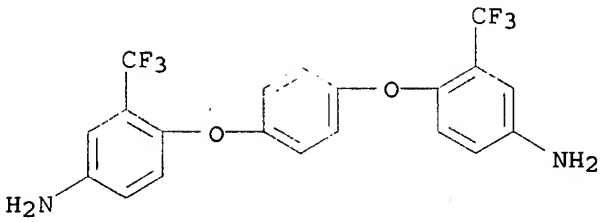
PAGE 1-B



RN 330160-46-8 CAPLUS
CN 1,3-Isobenzofurandione, 5,5'-oxybis-, polymer with 4,4'-[1,4-phenylenebis(oxy)]bis[3-(trifluoromethyl)benzenamine] (9CI) (CA INDEX NAME)

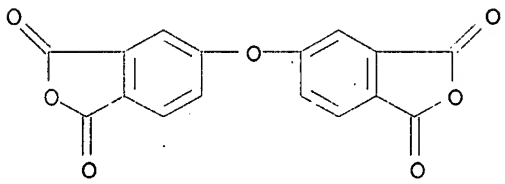
CM 1

CRN 94525-05-0
CMF C20 H14 F6 N2 O2

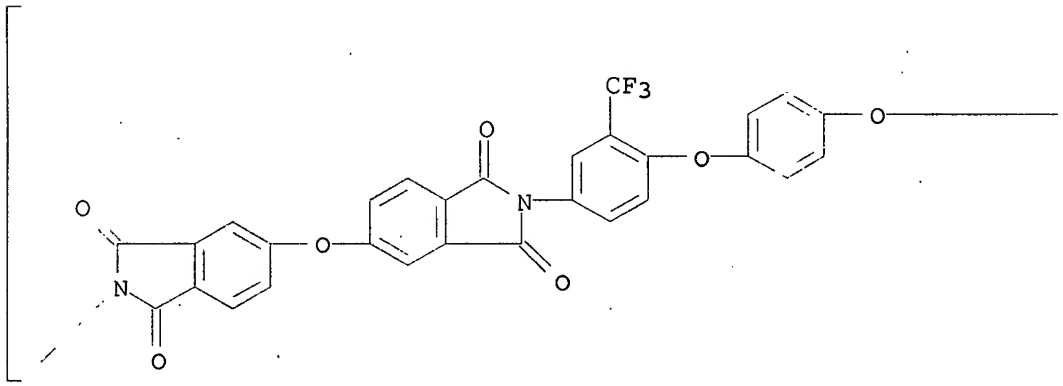


CM 2

CRN 1823-59-2
CMF C16 H6 O7



RN 330160-47-9 CAPLUS
CN Poly[(1,3-dihydro-1,3-dioxo-2H-isoindole-2,5-diyl)oxy(1,3-dihydro-1,3-dioxo-2H-isoindole-5,2-diyl)[3-(trifluoromethyl)-1,4-phenylene]oxy-1,4-phenyleneoxy[2-(trifluoromethyl)-1,4-phenylene]] (9CI) (CA INDEX NAME)



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REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

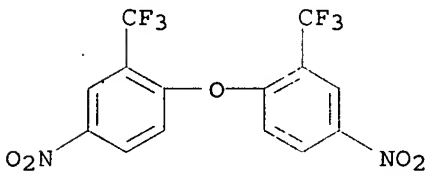
L9 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1961:137078 CAPLUS
DOCUMENT NUMBER: 55:137078
ORIGINAL REFERENCE NO.: 55:25775f-i,25776a-d
TITLE: Fluorinated aromatic amino acids. II. 2- and 3-Trifluoromethyltyrosines. Hydrolytic stability of the trifluoromethyl group on the aromatic nucleus
AUTHOR(S): Filler, Robert; Novar, Herman
CORPORATE SOURCE: Illinois Inst. of Technol., Chicago
SOURCE: Journal of Organic Chemistry (1961), 26, 2707-10
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 55:137078

AB cf. CA 54, 24520h. 2-Trifluoromethyl-DL-tyrosine (I) was prepared (17%) by the reaction of 2-trifluoromethyl-4-hydroxybenzenediazonium chloride (II) with acrylic acid (III), followed by ammonolysis. Attempts to prepare I via the azlactone route failed. 3-Trifluoromethyl-DL-tyrosine (IV) could not be prepared by either of these ways, although 3-trifluoromethyl-4-methoxy-DL-phenylalanine (V) was obtained in impure form by the Meerwein route. The critical factor in the failure to synthesize IV was the hydrolytic instability (in both acid and alkaline solution) of the trifluoromethyl group o- to an OH group. o-Chlorobenzotrifluoride (100 g.), 150 cc. H_2SO_4, and 100 cc. HNO_3 stirred 18 hrs. gave 109 g. 2-chloro-5-nitrobenzotrifluoride (VI), b8 100°, n30D 1.5031. VI (50 g.) in 150 cc. 95% alc. reduced by H (0.1 g. PtO_2, mixture shaken 3 hrs. at room temperature) gave 33 g. 2-chloro-5-aminobenzotrifluoride, b5 106°, n24.5D 1.5118. VI (10 g.) refluxed 5 hrs. with 6N KOH, acidified, and recrystd. gave 5-nitrosalicylic acid (VIa), m. 225-8°. When the conditions of this reaction were varied, no reaction occurred or the same product was obtained. 2-Hydroxy-5-nitrobenzotrifluoride (VII) was not detected. VI (45.2 g.) added dropwise to a solution of NaOMe (from 4.6 g. Na in 100 cc. MeOH) and the mixture stirred overnight at room temperature and acidified gave 38 g. 2-methoxy-5-nitrobenzotrifluoride (VIII), m. 79-9.5° (95% alc.). VI (80 g.) added to 50 g. KOH in 400 cc. MeOH, the mixture stirred 15 min. at room temperature, 6N HCl added, and the mixture cooled gave 75 g. VIII. VIII in AcOH refluxed 4 days with 48% HBr, the mixture extracted with Et_2O, and the extract evaporated and worked up gave VIa. VIII (7 g.) in 100 cc. 95% alc. reduced by H over 0.5 g. 5% Pd-C gave 4.9 g. 2-methoxy-5-aminobenzotrifluoride (IX), m. 59-60°. IX.HCl mixed with excess

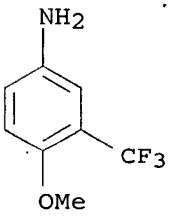
48% HBr and treated at 0° with aqueous NaNO2 gave 2-methoxy-5-bromobenzotrifluoride, b30 120°, n42D 1.4907. VI (75 g.) shaken 18 hrs. at 100° with liquid NH3 in a bomb gave 62 g. 2-amino-5-nitrobenzotrifluoride (X), m. 91.5-3.0° (C6H6-ligroine). X was converted to 2-bromo-5-nitrobenzotrifluoride via the Sandmeyer reaction (b12 125-30°, n38D 1.5263). X (21 g.) with 50 cc. concentrated H2SO4 and 100 cc. H2O treated at -5° with 7 g. NaNO2 in 20 cc. H2O, stirred overnight at room temperature, and extracted with Et2O gave an orange solid, m. 172.5-4.0°. VI (42 g.) added dropwise to 10 g. Na in 200 cc. PhCH2OH, the mixture stirred 1 hr. at room temperature and acidified, the solid in 150 cc. Et2O extracted with 5% NaOH, the Et2O evaporated, and solid crystallized gave 33 g. 2,2'-bistrifluoromethyl-4,4'-dinitrodiphenyl ether, m. 141-1.5°. The expected product, the benzyl ether of VII, was not detected. 2-Nitro-5-hydroxybenzotrifluoride (40 g.) in 100 cc. 95% alc. reduced by H (0.5 g. 5% Pd-C) and the mixture shaken 3 hrs. at room temperature and evaporated gave 29.5 g. 2-amino-5-hydroxybenzotrifluoride (XI), m. 154.5-5.5° (95% alc.). NaOAc (8.5 g.), 3 g. CuCl, 7.2 g. III, and 75 cc. Me2CO treated in a dry ice-Me2CO bath with a mixture of II (prepared from 20 cc. concentrated HCl and 10 cc. H2O with 17.7 g. XI previously treated with 7 g. NaNO2 in 20 cc. H2O), the mixture stirred 4 hrs. at room temperature and shaken with Et2O and H2O, the aqueous layer discarded, then washed with 10% NaOH, and the alkaline solution acidified and evaporated gave a residue after removal of III. This residue dissolved in 300 cc. concentrated NH4OH, the mixture shaken 4 days at room temperature, heated on a steam bath, concentrated, and treated with 95% alc., and the product precipitated gave 4.25 g. I, m. 212-25° (decomposition).

IT 344-47-8P, Ether, bis(α,α,α-trifluoro-4-nitro-o-tolyl) 393-15-7P, p-Anisidine, 3-(trifluoromethyl)- 654-76-2P, Anisole, 4-nitro-2-(trifluoromethyl)- 1514-11-0P, Anisole, 4-bromo-2-(trifluoromethyl)-
RL: PREP (Preparation)
(preparation of)

RN 344-47-8 CAPLUS
CN Benzene, 1,1'-oxybis[4-nitro-2-(trifluoromethyl)- (CA INDEX NAME)



RN 393-15-7 CAPLUS
CN Benzenamine, 4-methoxy-3-(trifluoromethyl)- (CA INDEX NAME)



RN 654-76-2 CAPLUS